UCRL-JC-119469 Abs

Abstract Submitted
for the Mar95 Meeting of
The American Physical Society

Sorting Category: 7c

Intrinsic Point Defects in B32 LiAl C. WOODWARD, *UES, Inc.*, R. BENEDEK, *Argonne National Laboratory,* S.A. KAJIHARA, *NRC Associate, Wright Lab.,* L.H. YANG*, *Lawrence Livermore National Lab.* ---- Point defects in the Zintl-phase intermetallic compound LiAl have been investigated extensively owing to the possible application of this alloy as an electrode material in high energy density batteries. An important feature of this system is the large concentration of constitutional vacancies even at ideal stoichiometry. Relaxed structures and energies for vacancy and antisite defects were calculated for Zintl phase (B32) LiAl within the local density functional theory framework using a plane-wave-pseudopotential treatment and a conjugate gradient diagonalization procedure. A quasi-Newton method was employed to optimize the atomic coordinates. Supercell sizes of 16, 64 and 128 atom with 20, 70, and 132 electron bands respectively, were employed. Estimates for the equilibrium defect concentration as a function of temperature and composition will be presented.
*Work at LLNL was performed under auspices of U.S. DoE under Contract No. W-7405-ENG-48.